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Publications and Summaries of Work

1. *Continuation – Conjugate Gradient Methods For The Least Squares Solution of Nonlinear Boundary Value Problems*, R. Glowinski, H.B. Keller and L. Reinhart, SIAM J. Sci. Stat. Compt., V.6, No.4, October 1985 (793-832).

We discuss in this paper a new combination of methods for solving nonlinear boundary value problems containing a parameter. Methods of the continuation type are combined with least squares formulations, preconditioned conjugate gradient algorithms and finite element approximations. We can compute branches of solutions with limit points, bifurcation points, etc.

Several numerical tests illustrate the possibilities of the methods discussed in the present paper; these include the Bratu problem in one and two dimensions, one-dimensional bifurcation and perturbed bifurcation problems, the driven cavity problem for the Navier-Stokes equations.

2. *Some bifurcation diagrams for Taylor vortex flows*; Rita Meyer-Spasche and H.B. Keller, Phys. Fluids 28 (5), May 1985 (1248–1252).

The numerical continuation and bifurcation methods of Keller [H.B. Keller, in *Applications of Bifurcation Theory* (Academic, New York, 1977), pp. 359–384] are used to study the variants of some branches of axisymmetric Taylor vortex flow as the wavelength in the axial direction changes. Closed "loops" of solutions and secondary bifurcations are determined. Variations with respect to Reynolds number show the same phenomena. The results presented here show that Taylor vortices with periodic boundary conditions exist in a wider range of wavelengths, λ, than observed in the Burkhalter/Koschmieder experiments [Phys. Fluids 17, 1929 (1974)]. They also show that there is possibly a λ subinterval within the neutral curve of Couette flow such that there are no Taylor vortex flows with smallest period in this interval.

3. *A Direct Method For Computing Higher Order Folds*, Zhong-Hua Yang and H.B. Keller, SIAM J. Sci. Stat. Comput., V.7, No.2, April 1986 (351–361).

We consider the computation of higher order fold or limit points of two parameter-dependent nonlinear problems. A direct method is proposed and an efficient implementation of the direct method is presented. Numerical results for the thermal ignition problem are given.

A-1

4. *Exact Boundary Conditions At An Artificial Boundary For Partial Differential Equations In Cylinders*, Thomas Hagstrom and H.B. Keller, SIAM J. Math. Anal., V.17, No.2, March 1986 (322–341).

The numerical solution of partial differential equations in unbounded domains requires a finite computational domain. Often one obtains a finite domain by introducing an artifical boundary and imposing boundary conditions there. This paper derives exact boundary conditions at an artificial boundary for partial differential equations in cylinders. An abstract theory is developed to analyze the general linear problem. Solvability requirements and estimates of the solution of the resulting finite problem are obtained by use of the notions of exponential and ordinary dichotomies. Useful representations of the boundary conditions are derived using separation of variables for problems with constant tails. The constant tail results are extended to problems whose coefficients obtain limits at infinity by use of an abstract perturbation theory. The perturbation theory approach is also applied to a class of nonlinear problems. General asymptotic formulas for the boundary conditions are derived and displayed in detail.

5. *The Numerical Calculation Of Traveling Wave Solutions Of Nonlinear Parabolic Equations*; Thomas Hagstrom and H.B. Keller, SIAM J. Sci. Stat. Comput., V.7, No.3, July 1986 (978–988).

Traveling wave solutions have been studied for a variety of nonlinear parabolic problems. In the initial value approach to such problems the initial data at infinity determines the wave that propagates. The numerical simulation of such problems is thus quite difficult. If the domain is replaced by a finite one, to facilitate numerical computations, then appropriate boundary conditions on the "artificial " boundaries must depend upon the initial data in the discarded region. In this work we derive such boundary conditions, based on the Laplace transform of the linearized problems at $\pm\infty$, and illustrate their ability by presenting a numerical solution of Fisher's equation which has been proposed as a model in genetics.

6. *A Multigrid Continuation Method For Elliptic Problems With Folds*; John H. Bolstad and Herbert B. Keller, SIAM J. Sci. Stat. Comput., V.7, No.4, October 1986 (1081–1104).

We introduce a new multigrid continuation method for computing solutions of nonlinear elliptic eigenvalue problems which contain limit points (also called turning points or folds). Our method combines the frozen tau technique of Brandt with pseudo-arc length continuation and correction of the parameter on the coarsest grid. This produces considerable storage savings over direct continuation methods, as well as better initial coarse grid approximations, and avoids complicated algorithms for determining the parameter on finer grids. We provide numerical results for second, fourth and sixth order approximations to the two-parameter, two-dimensional stationary reaction-diffusion problem:

$$\Delta u + \lambda \exp(u/(1 + \alpha u)) = 0.$$

For the higher order interpolations we use bicubic and biquintic splines. The convergence rate is observed to be independent of the occurences of limit points.

7. *Multiple Laminar Flows Through Curved Pipes*, Zhong-hua Yang and H.B. Keller, Applied Numerical Mathematics 2, North Holland, 1986 (257–271).

The Dean Problem of steady viscous flow through a coiled circular pipe is studied numerically for a large range of Dean number and for several coiling ratios. We find that the solution family, as parameterized by Dean number, has numerous folds or limit points. Four folds and hence five branches of solutions are found. We speculate that infinitely many solutions can exist in this family for some fixed value(s) of D. More resolution and higher accuracy would be required to justify our conjecture and to find the rule of formation of new solution branches.

8. *Asymptotic Boundary Conditions and Numerical Methods for Nonlinear Elliptic Problems on Unbounded Domains*. T.M. Hagstrom and H.B. Keller, Mathematics of Computation, V.48, No.178, 1987 (449–470).

We present a derivation and implemesntation of asymptotic boundary conditions to be imposed on "artificial " boundaries for nonlinear elliptic boundary value problems on semi-infinite "cylindrical" domains. A general theory developed by the authors in [11] is applied to establish the existence of *exact* boundary conditions and then to obtain useful approximations to them. The derivation is based on the Laplace transform solution of the linearized problem at infinity. We discuss the incorporation of the asymptotic boundary conditions into a finite-difference scheme and present the results of numerical experiments on the solution of the Bratu problem in a two-dimensional stepped channel. We also touch on certain problems concerning the existence of solutions of this problem on infinite domains and conjecture on the behavior of the critical parameter value with respect to changes in the domain. Some numerical evidence supporting the conjecture is given.

9. *Computation Of Anomalous Modes in the Taylor Experiment*. J.H. Bolstad and H.B. Keller, Journal of Computational Physics, V.69, No.1, March 1987 (230–251).

Multigrid continuation methods are used to solve the steady, axisymmetric incompressible Navier-Stokes equations for Taylor-Couette flows between cylinders of finite or infinite length. Using Schaeffer's homotopy, we compute (for finite cylinders) anomalous modes (those seeming to have an odd number of vortices, or seeming to have the "wrong" direction of rotation at an endplate). The results show that these modes possess extra vertices not observed in the experiments of Benjamin and Mullin (*Proc. Roy. Soc. London Ser. A*377 (1981), 221: *J. Fluid Mech.* 121 (1982), 219). Our computations verify conjectures of Schaeffer, and of Benjamin and Mullin on the unfolding of the bifurcation diagram as periodic (infinite cylinder) flows are continuously transformed to flows with rigid ends. We obtain five distinct solutions with the same Reynolds number, aspect ratio, and radius ratio, and give a systematic procedure for obtaining them. The numerical results show quanitative agreement with the more recent experiments of Cliffe and Mullin (*J. Fluid Mech.* 153 (1985), 243).

10. *Equilibrium Chaos And Related Parameter Sequences*; H.B. Keller and J.M. Fier, Analyse Mathematique et Applications, Gauthier-Villars, Paris, 1988 (235–244).

We consider some equilibrium phenomena depending upon on one or more parameters which have the property that an infinite sequence of equilibrium states exist for finite parameter values. Viewing the solution manifold as a path in an appropriate space we see that the path has an infinite number of folds. At these limit points or folds the number of solutions or equilibrium states changes by two - either gained or lost. This is vaguely similar to the period doubling phenomenon that occurs in various dynamical systems or more simply in the Lorenz map. This has led us to conjecture that the difference quotients of the parameter values at which the folds occur approach "universal" limits. We show here, in several cases, that they indeed do converge to limits but that the limits are far from universal.

We actually obtain these limits and show how they vary with other parameters in the problems. A similar analysis may be possible for some dynamical systems. The crucial step is to be able to find an appropriate plane in which a phase plane analysis can be carried out.

11. *Computations of Taylor Vortex Flows Using Multigrid Continuation Methods*, Nathan Dinar and Herbert B. Keller, (to be submitted).

Numerical solutions of axisymmetric Taylor vortex flows have been calculated using Multigrid Continuation Techniques. Both infinite and finite cylinders are considered, and the results agree well with experiments. New solutions are found in the infinite cylinder case and these, surprisingly, may help in understanding some experimental results obtained in relatively short cylinders. The numerical method proved to be efficient and reliable so that computations with fine grids and long cylinders are easily performed.

12. *Complex Bifurcation From Real Paths* . M. Henderson and H.B. Keller, SIAM J. Appl. Math.(to appear).

We study a new bifurcation phenomenon which we call complex bifurcation. The basic idea is simply that real solution paths of real analytic problems frequently have complex paths bifurcating from them. Indeed the phenomenon is not rare since it occurs at fold points, at pitchfork bifurcation points and at isola centers. If the problem of interest is finite dimensional with nonlinear algebraic equations then our observation is simply that real roots may become complex as some parameter varies. Thus indeed discrete approximations of nonlinear functional equations frequently exhibit this phenomenon. However, these discrete complex paths need not be spurious since, as we show, the underlying problem in a Banach space setting also exhibits the same behavior.

13 *Diffusive Fronts Of Penetrants In Glassy Polymers*, Donald S. Cohen, Physica 12D, North Holland, Amsterdam, 1984 (369-374).

A model for diffusion in polymers near the glass-rubber transition is developed. The model unifies many of the diverse observations made in various kinds of glassy polymers. Preliminary studies of the diffusive penetrant front are carried out.

14 *Chemical Reactor Theory And Problems In Diffusion*, Donald S. Cohen and Roger Alexander, Physica 20D, North-Holland, Amsterdam, 1986 (122–141).

A survey of selected results and new problems involving classical and non-classical diffusion is presented. The classical results are given via reaction-diffusion equations modeling stirred tank and tubular chemical reactors. The more recent diffusive phenomena arise in several contexts; we shall use liquid and gaseous penetration in polymers to illustrate the observations.

15 *Sorption Of A Finite Amount Of Swelling Solvent In A Glassy Polymer*; Donald S. Cohen and Charles Goodhart, Journal of Polymer Science: Part B: Polymer Physics, V.25, 1987 (611–617).

We study the time history of a diffusing front when a polymer is exposed to a finite amount of penetrant which becomes used up. A class of polymers is considered for which slow molecular relaxation occurs only at or near the glass-gel interface with instantaneous relaxation both ahead of and behind the progressing front. We show that the position of the penetrant front versus time undergoes a long smooth transition from standard Fickian $t^{1/2}$ behavior to exponential time decay onto a final equilibrium position attained when all the penetrant is used up.

16 *Asymptotic Methods of Semi – Conductor Modeling*. Donald S. Cohen, M.J. Ward and F.M. Odeh, NASECODE V Conference Proceedings, Trinity College, Dublin, Ireland, Boole Press Dublin, 1987 (333–339).

In this note a brief summary of an asymptotic study of the semiconductor equations relevant to a long n-channel MOSFET is presented. Using formal asymptotic techniques, a pointwise description of the potential and the carrier concentration is obtained. From this description, an asymptotic expression for the mobile charge *uniform* across the weak-strong invesrsion transition, which is needed for device characteristics, is available.

17 *Free Boundary Problems In Controlled Release Pharmaceuticals Diffu–sion In Glassy Polymers*, Donald S. Cohen and Thomas Erneux, SIAM J. Appl. Math.(to appear).

We formulate and study two different problems occurring in the formation and use of pharmaceuticals via controlled release methods. These problems involve a glassy polymer and a penetrant, and the central problem is to predict and control the diffusive behavior of the penetrant through the polymer. Our mathematical theory yields free boundary problems which we study in various asymptotic regimes.

18 *Free Boundary Problems In Controlled Release Pharmaceuticals Swelling Controlled Release*, Donald S. Cohen and Thomas Erneux, SIAM J. Appl. Math.(to appear).

We formulate and study a problem in controlled release pharmaceutical systems. The device we model is a polymer matrix containing an initially immobilized drug. The release of the drug is achieved by countercurrent diffusion through a penetrant solvent with the release rate being determined by the rate of diffusion of the solvent in the polymer. Our mathematical theory yields a free boundary problem which we study in various asymptotic regimes.

19 *A Mathematical Model For Stress – Driven Diffusion In Polymers*, Robert W. Cox and Donald S. Cohen, J. Polymer Science:Physics Edition (to appear).

A model for Case II diffusion into polymers is presented. The addition of stress terms to the Fickian flux is used to produce the characteristic progressive front. The stress in turn obeys a concentration dependent evolution equation. The model equations are analyzed in the limit of small diffusivity for the problem of penetration into a semi-infinite medium. Provided that the coefficient functions obey two monotonicity conditions, the solvent concentration profile is shown to have a steep front that progresses into the medium. The formulas governing the progression of the front are developed. After the front decays away, the long time behavior of the solution is shown to be a similarity solution as in Fickian diffusion. Two techniques for approximating the solvent concentration and the front position are presented. The first approximation method is a series expansion; formulas are given for the initial speed and deceleration of the front. The second approximation method uses a portion of the long time similarity solution to represent the short time solution behind the front.

Ph.D. Degrees Awarded in Related Research

The following people worked on this program while graduate students and obtained their Ph.D. degrees in Applied Mathematics at Caltech. Their thesis titles are listed.

1 J.M. Fier,1985, (Advisor: H.B. Keller)
I: *Fold Continuation and the Flow Between Rotating Coaxial Disks.*
II: *Equilibrium Chaos.*
III. *A Mesh Selection Algorithm for Two – Point Boundary Value Problems.*

2 Mary Elizabeth Brewster, 1987 (Advisor: H.B. Keller)
I: *Asymptotic Analysis of Thin Plates Under Normal Load and Horizontal Edge Thrust.*

3 Tomas Paul Girnius, 1986 (Advisor: H.B. Keller)
I: *Ray Tracing in Complex Three – Dimensional Earth Models.*

4 Michael E. Henderson, 1985 (Advisor: H.B. Keller)
I: *Complex Bifurcation.*

5 Elizabeth Ann Stanley, 1985 (Advisor: D.S. Cohen)
I: *Diffusion in Glassy Polymers*,

6 Donald William Schwendeman, 1986 (Advisor: G.B. Whitham)
I: *Numerical Shock Propagation Using Geometrical Shock Dynamics*

7 Michael J. Ward, 1988 (Advisor: D.S. Cohen)
I: *Asymptotic Methods in Semiconductor Device Modeling.*

8 Robert W. Cox, 1988 (Advisor: D.S. Cohen)
I: *A Model for Stress – Driven Diffusion in Polymers.*

Other Personnel Supported by this Program.

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